

Phases of attractive spin-imbalanced fermions in square optical lattices

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We determine the relative stability of different ground-state phases of spin-imbalanced populations of attractive fermions in square lattices. The phases are systematically characterized by the symmetry of the order parameter and the real- and momentum-space structures using Hartree-Fock-Bogoliubov theory. We find several type of unidirectional Larkin-Ovchinnikov-type phases. We discuss the effect of commensuration between the ordering wave vector and the density imbalance, and describe the mechanism of Fermi surface reconstruction and pairing for various orders. A robust supersolid phase is shown to exist when the ordering wave vector is diagonally directed.

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There has been a surge of interest in the possibility of realizing unconventional fermionic superfluids using cold atomic gases. Amongst the many possibilities offered by the highly tunable Hamiltonians available in cold-atoms experiments, the simplest remains that of a two-component density-imbalanced populations of fermions with attractive interactions. The theoretical study of such systems dates back to Fulde and Ferrel (FF) [1] and Larkin and Ovchinnikov (LO) [2] who independently suggested that the mismatch between the Fermi surfaces of the two species could result in the formation of a condensate of finite-momentum pairs. Atomic gases offer a direct route to the realization of FFLO phases, circumventing most of the difficulties of solid state systems, thanks to the possibility of controlling independently the density of the two species, the absence of disorder and, most importantly, the ability to engineer strong interactions. In spite of this, the existence of an FFLO phase in two and three dimensions has been argued to be confined to a small range of interaction strengths and polarizations[3], and detection has remained elusive.

The possibility of using optical lattices has been suggested by several authors[4, 5] as a key ingredient to observe FFLO-type states. The best empirical indication that this may be the case is provided by experiments on strongly-correlated-electrons materials and the fact that, when doped, these systems show a tendency toward formation of inhomogeneities in the form of spin, charge and, possibly, pairing density waves. The relevance of these experiments to the properties of attractive fermions in optical lattices stems from the belief that, in both cases, the essential physics can be captured by a one-band Hubbard model: with an on-site repulsive interaction for many of the electronic systems and an on-site attraction in an optical lattice. The attractive and repulsive cases are mapped into each other by a particle-hole transformation[4] and the presence of spin-texture in the doped repulsive case translates into the occurrence of a modulated superfluid in an imbalanced population of attractive fermions, *i.e.* an FFLO phase. This is reinforced by recent quantum Monte Carlo results [6] on the two-dimensional repulsive model showing spin-density waves

with long wavelength modulation.

Despite this mapping and several works addressing the existence of a possible FFLO phase [7–9], the nature of the ground state phases in a spin-imbalanced two-dimensional optical lattice remains largely undetermined. On the one hand, information on the repulsive model is entirely confined to the case of unpolarized systems, which maps into the attractive case at half-filling: $n_{\uparrow} + n_{\downarrow} = 1$; for the case of imbalanced fermionic population, one is interested in the more general case of a polarized system and arbitrary density. On the other hand, works addressing the physics in the lattice have either focused on the single plane-wave form of the order parameter[7, 8], which is likely incorrect at low temperature[2], or on selected states[9] (*e.g.* fixed modulation wavelength) because of the challenge of removing large finite-size effects.

In this paper, we determine systematically the ground state phases of the attractive two-dimensional spin-imbalanced optical lattice system away from half-filling. Within mean-field theory, we converge the numerical calculations to the thermodynamic limit, and characterize the order parameter and the real- and momentum-space properties for different densities and polarizations. Small to moderate interaction strengths are considered, where mean-field theory is expected to capture the correct physics. We find the existence of several types of LO phases in a large region of the parameter space, with distinct physical characteristics which have not been described before. Particularly noteworthy is a robust supersolid phase obtained when the ordering wave vector is directed along the diagonal direction.

Results presented in this work are obtained using Hartree-Fock-Bogoliubov theory so that modulations in charge, spin and pairing are all handled on the same footing. The starting Hamiltonian reads

$$H = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} - U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu n_i - \frac{\hbar}{2} m_i, \quad (1)$$

where $c_{i\sigma}$ are fermionic annihilation operators of spin σ on site i , $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$, $n_i = n_{i\uparrow} + n_{i\downarrow}$, $m_i = n_{i\uparrow} - n_{i\downarrow}$.

In order to accommodate the inhomogeneities, the calculations are performed on finite simulation cells whose shape is dictated by the symmetry of the targeted phase. The cells are characterized by two basis vectors, L_1 and L_2 , whose components are integers. Once the cell shape is chosen, we define Bloch states as $c_j(k) \propto \sum_L c_{j+L} \exp[ik \cdot L]$ where $L = n_1 L_1 + n_2 L_2$, and k is a vector that varies freely within the first BZ of the reciprocal lattice. Then, using these states and the mean-field approximation, the Hamiltonian decouples into a sum of k -dependent pieces, $H = \sum_k H(k)$, of the form

$$H(k) = [\mathbf{c}_\uparrow^\dagger \mathbf{c}_\downarrow] \begin{bmatrix} \mathbf{H}_\uparrow(k) & \mathbf{\Delta} \\ \mathbf{\Delta}^\dagger & -\mathbf{H}_\downarrow(G-k) \end{bmatrix} [\mathbf{c}_\uparrow \mathbf{c}_\downarrow^\dagger]^T, \quad (2)$$

where \mathbf{c}_\uparrow and \mathbf{c}_\downarrow represent an array (row) of operators, $\{c_{i\uparrow}(k)\}$ and $\{c_{i\downarrow}(G-k)\}$ respectively, with index i running over the N sites of the simulation cell, and G is defined below. \mathbf{H} and $\mathbf{\Delta}$ are $N \times N$ matrices with elements

$$\begin{aligned} [\mathbf{H}_\sigma(k)]_{ij} &= -t_{ij}(k) + \delta_{ij}(D_{i\sigma} - \mu - s_\sigma h/2) \\ [\mathbf{\Delta}(k)]_{ij} &= \delta_{ij} \Delta_i. \end{aligned} \quad (3)$$

In the above, $t_{ij}(k) = \sum_L \exp(ik \cdot L) t_{i,j+L}$, $s_{\uparrow/\downarrow} = \pm 1$ and $D_{i\sigma}$, Δ_i , μ and h are determined by the requirement that the Free energy $F = \langle H \rangle - TS$ is a minimum for the target average densities n_σ . This amounts to the following self-consistency equations

$$\begin{aligned} D_{i-\sigma} &= U \int dk \langle c_{i\sigma}^\dagger(k) c_{i\sigma}(k) \rangle, \\ \Delta_i &= -U \int dk \langle c_{i\sigma}^\dagger(k) c_{i-\sigma}^\dagger(k) \rangle, \\ \bar{n}_\sigma &= N^{-1} \sum_i \int dk \langle c_{i\sigma}^\dagger(k) c_{i\sigma}(k) \rangle, \end{aligned} \quad (4)$$

with expectation values evaluated in the simulation cell.

The variable G in Eq. (2) is a vector such that $\theta = G \cdot L$ gives the twist angle of the pairing order parameter under translation by L . For collinear phases, θ is either 0 or π , giving periodic or anti-periodic boundary conditions on $\langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \rangle$. Note that uniform phases with a spiral order parameter (FF type) amount to the choice of a one-site cell and a G equal to the wave-vector of the spiral modulation. Thus $H(k)$ is specified by a 2×2 matrix, and the eigenvalues and eigenvectors can be computed analytically. in the spiral phase[1].

Given a set of symmetry-equivalent q vectors, linear response theory can be used to show that the onset of instabilities of the form

$$\Delta_i = \sum_q \Delta_q e^{iq \cdot r_i}, \quad (5)$$

must happen at exactly the same value of U , regardless of the choice of Δ_q . In order to determine the correct

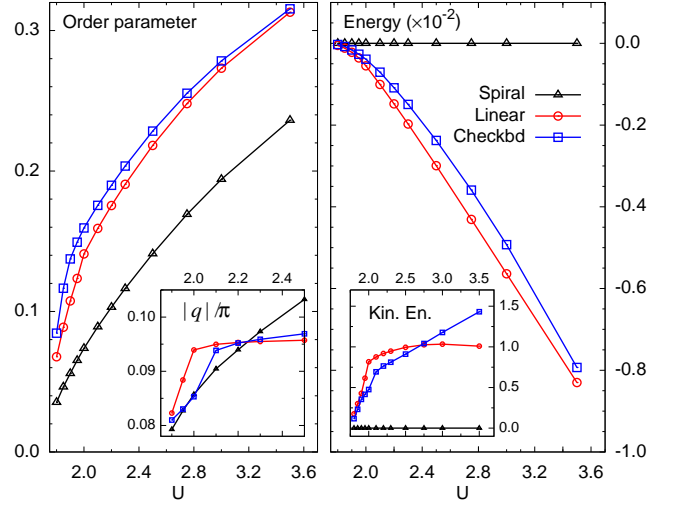


FIG. 1: Left Panel: local order parameter, $\max_i |\langle c_{i\uparrow} c_{i\downarrow} \rangle|$, and leading wavevector (inset) versus U for $\langle c_{i\uparrow} c_{i\downarrow} \rangle \propto e^{iq_x \cdot r_i}$ (Spiral), $\langle c_{i\uparrow} c_{i\downarrow} \rangle \propto \cos(q_x \cdot r_i)$ (Linear), $\langle c_{i\uparrow} c_{i\downarrow} \rangle \propto \cos(q_x \cdot r_i) + \cos(q_y \cdot r_i)$ (Checkbd) with $q_x = |q|(1, 0)$ and $q_y = |q|(0, 1)$. Right panel: relative energies (units of t) of the three phases.

form of order parameter, we proceed as follows. We first determine U_c and the associated non-zero wave-vector q_c using the single plane-wave form as this allows for a quick exploration of phase space. We find that q_c is directed along any of the four, symmetry-equivalent directions $(\pm 1, 0)$, $(0, \pm 1)$ and, therefore, any linear combination of the four associated plane waves is a candidate ground state order parameter just above U_c . To resolve which one leads to the largest lowering of energy, we proceed by solving the mean-field equations for the three cases corresponding to spiral ($\Delta_i \propto \exp(iq_x \cdot r_i)$), unidirectional ($\Delta_i \propto \cos(q_x \cdot r_i)$) and checkerboard ($\Delta_i \propto \cos(q_x \cdot r_i) + \cos(q_y \cdot r_i)$) pairing density wave and track the evolution of $|q|$ as a function of U . Explicit calculations in large simulation cells on the repulsive model (with simulated annealing starting with random initial fields[10]) have shown that instabilities involving q -vectors in different, non-equivalent directions, which the above approach would miss, are unlikely to occur in the range of U considered here.

Mean-field results[10] on the repulsive model and the particle-hole transformation relating the attractive and repulsive models imply the existence of the following properties at half-filling, i.e., when the average particle density is precisely one fermion per site: 1) a critical U exists such that, above it, the system develops a phase with an inhomogeneous order parameter 2) the pairing order parameter is characterized by a wave vector $|q| = m\pi$ where $m = n_\uparrow - n_\downarrow$ is the average magnetization 3) both fermionic species have a gap in their single particle spectrum 4) as U grows larger there is a transition from a pair-density-wave in the $(1, 0)$ state to one in

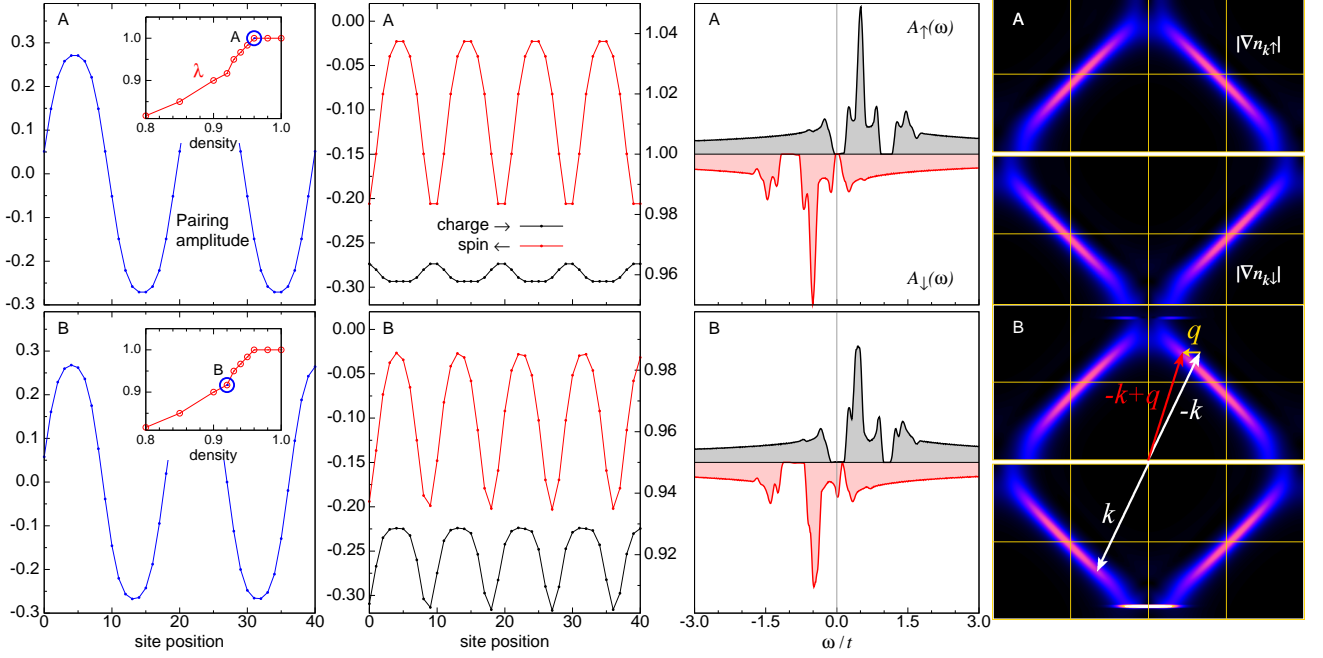


FIG. 2: Local properties and gradient of the momentum distribution for $n_{\uparrow} - n_{\downarrow} = -0.05$ at two densities: (A) $n = 0.96$ (top row) and (B) $n = 0.93$ (bottom). In both cases, the finite-momentum of the pair, q , is in the (1,0)-direction. The inset in the first column shows the evolution of $\lambda = m\pi/q$ as a function of density; case A belongs to the commensurate regime with unit density of excess-spin particles per node, while case B is in the incommensurate regime. The third column is the local density of state measured at site 0. In the fourth column, each panel shows two halves of the Fermi surface, for the \uparrow (minority) and \downarrow (majority) spins, respectively. The arrows in the figure indicate the pairing construction and applies to every pair across the FS, leading to one common q .

the (1,1) direction 5) order can be arbitrarily broken into a charge or a pairing instability or a combination of the two. This last point is a consequence of the possibility of breaking spin symmetry in any of the three equivalent direction in the repulsive case. It implies that charge and pairing orders compete, in the sense that the larger one is, the smaller the other must be.

We next present results away from half-filling. Figure 1 shows that the ground state has unidirectional LO order, with illustrative examples for $m \equiv n_{\uparrow} - n_{\downarrow} = -0.095$ and $n = 0.95$. The presence of the lattice is manifested as the significantly different shape of the non-interacting Fermi surfaces when compared to their circular counterparts in the continuum. Such differences are largest when $n_{\sigma} = 0.5$ and gradually disappear as the density is reduced. For this reason, we repeat a similar analysis in different regimes of density and polarization, $n = 0.95, 0.75$ and 0.5 and $m/n = 0.1$ and 0.4 , so as to have a rather complete picture close and away from half-filling, at small and large polarization and in an interaction range that extends from U_c up to $U = 4$. The results are summarized in Table I. These are consistent with earlier results addressing the physics of FFLO phases in the continuum, which found checkerboard order close to U_c thanks to an expansion in powers of the order parameter[11], but show

m/n	$n = 0.95$	$n = 0.75$	$n = 0.5$
0.1	$U_c = 1.8$	$U_c = 1.8$	$U_c = 2.0$
	$q_c = 0.071\pi$ L; L	$q_c = 0.078\pi$ L; L	$q_c = 0.066$ C; L
0.4	$U_c = 3.6$	$U_c = 3.2$	$U_c = 2.8$
	$q_c = 0.34\pi$ L; L	$q_c = 0.30\pi$ L; L	$q_c = 0.27\pi$ C; C

TABLE I: Critical parameter at the onset of order for a few densities (n) and polarizations (m/n). The wavevector is directed along (1,0). The two letters in last line in each table cell describe the type of order just above U_c and at $U = 4$, respectively (L=linear, C=checkerboard).

that for $n \geq 0.75$ lattice effects are strong enough to return unidirectional order independently of polarization or proximity to U_c . Given the difficulty in observing unconventional pairing in the continuum, the latter is the density regime where an experimental realization of the FFLO state should be most feasible. We will therefore focus on it in the following.

Figure 2 characterizes the FFLO phase at $U = 3t$ and for $m = 0.05$ in two qualitatively different density regimes. In particular, for $n > 0.95$, the wave vector is precisely determined by the magnetization via the same

relation holding at half-filling, $q = m\pi$. This commensurate regime is characterized by a density of *one* excess particle per node (of the order parameter) and consequently band-insulating behavior along the node. This is most clearly seen in the local density of states at the node, with both species showing a gap at the Fermi energy. Correspondingly the gradient of the momentum distribution shows no sharp lines indicative of the existence of a Fermi surface. The commensurate regime here has, however, some important distinctions from half-filling. First, the interchangeability between pairing and charge orders is broken as soon as the average density deviates from $n = 1$, and pairing emerges as the dominant order. Second, the density is not perfectly uniform, as it is for the purely superfluid phase at half-filling. The density is instead characterized by a weak modulation that reflects the different degrees of localization of the Andreev states for the two spin species. The density profile shows weak peaks at the nodes indicating that the majority species has stronger localization.

In the second density regime, $n < 0.95$, the majority spin species develop a finite density of states at the nodes of the order parameter. Fermi arcs (sharp lines) are seen in $|\nabla n_{k\downarrow}|$. The arc in Fig. 2.B is of perfectly one-dimensional nature, indicating a complete decoupling between the metallic states living at different nodes. At larger polarization, the arcs will more strongly resemble the underlying Fermi surface of the non-interacting species. Finally, the density profile shows minima at the nodes, rather than the maxima observed in case A, as a direct consequence of the gradual emptying of the majority-spin Andreev bands visible in the local density of states. This is a potentially important experimental signature as it allows one to characterize the nature of the nodal metal via a static local property instead of a collective property such as the distance between nodes or the presence of Fermi arcs.

Next we consider the phases at larger interaction strengths U . Results on the repulsive model[10] indicate that the ordering wave vector switches to the $(1,1)$ direction at sufficiently small m and $U > 3t$. We focus on $U = 4t$ for an extensive and systematic examination of the properties of these phases. Indeed unidirectional LO states along the diagonal direction are found; however, we find that the system can accommodate both pairing and charge orders as *non-competing* instabilities away from half-filling. The real- and momentum-space properties of the phases are shown in Fig. 3. In contrast with the $(1,0)$ -direction paired state, pairing here is achieved by a reconstruction of the Fermi surface. The non-interacting surface of the majority spin is stretched, while that of the minority spin is compressed, along the $(-1,1)$ direction so that the reconstructed surfaces become “nested” via $k \rightarrow -k + q$ as illustrated in the middle row of Fig.3. The charge-density wave that develops at larger density is a consequence of the (π, π) nesting along the $(1,1)$ -

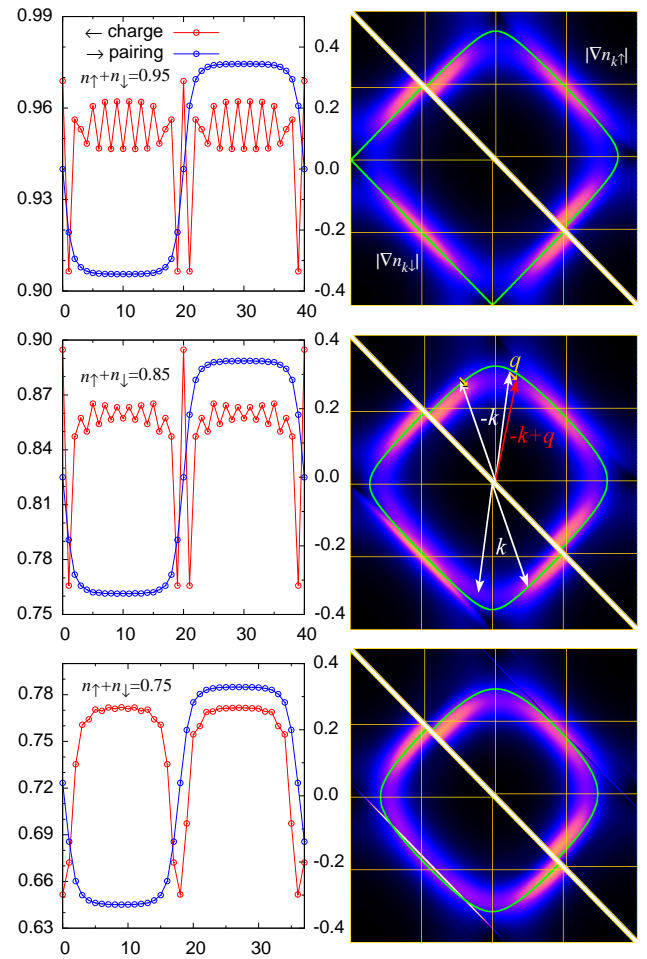


FIG. 3: Left panels: Evolution of charge and pairing order as density is reduced, for $m = 0.05$. Right panels: corresponding evolution of the gradient of the momentum distributions, and illustration of Fermi surface reconstruction and pairing. The pairing wave-vector, q , is in the $(-1,1)$ -direction. The solid (green) lines give the non-interacting Fermi surface.

direction which results from the reconstruction; its amplitude increases with the amount of nested states. The charge order is complementary to pairing, and further lowers the energy.

The new phase discussed above has an important distinction from the supersolid phase that can occur at half-filling. There both charge and pairing orders are associated with wave-vectors coupling the same regions around the Fermi surface: if pairing order happens at q , charge order must happen at $(\pi, \pi) - q$ and one can dial the form of the order parameter interpolating between a purely superfluid and a purely charge-density wave state. Here, away from half-filling, however, pairing is characterized by a polarization dependent wave-vector q while charge order appears at (π, π) and *cannot* be dialed away.

Our results are summarized in the phase diagram of Fig. 4 for $U = 3t$ and $U = 4t$. We found no evidence

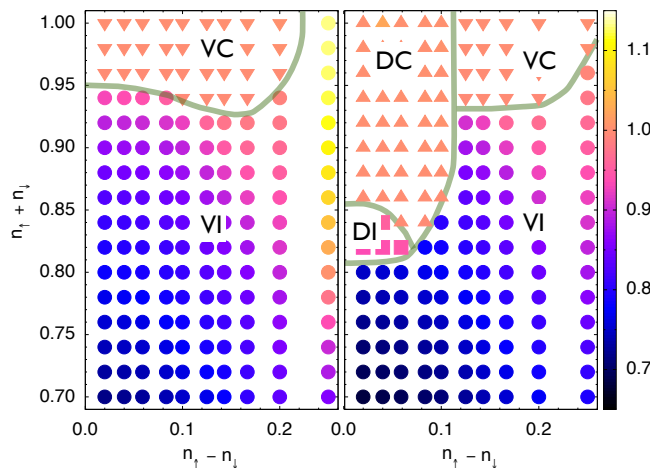


FIG. 4: $U/t = 3$ (left) and $U/t = 4$ (right) $T = 0$ phase diagram. The color axis reports values of $\lambda = m\pi/|q|$. Triangles represent the commensurate phases ($\lambda = 1$). Up-triangles have $q \propto (1, 1)$ (DC=Diagonal commensurate) while down-triangles have $q \propto (1, 0)$ (VC=Vertical Commensurate). Circles and square are Vertical and Diagonal Incommensurate phases (VI and DI).

of diagonal order at $U = 3t$. Its region of stability for the commensurate phase is limited to small polarization and density close to one. At $U = 4t$, the diagonal wave vector is almost always commensurate with m , and pairing and charge order coexist in all but a small fraction of the phase diagram where the diagonal phase is the correct ground state. This suggests that the charge-density wave play a small but important role in stabilizing diagonal order. Although the different symmetry between diagonal and vertical phases implies that the transition is discontinuous and accompanied by phase separation, we have not attempted an in-depth study of how this affects the situation at $U = 4t$. However, a simpler analysis based on considering phase separation in two phases having the same density and different magnetization leads to a narrow coexistence region ($\Delta m = 0.02$ at $n = 1$) and makes it sensible to assume that the broad feature of the phase diagram are, in fact, robust.

In summary, we have determined the type of phases that an imbalanced population of two fermionic species with attractive interactions support in the two-dimensional square lattice. Their real- and momentum-space properties are quantitatively characterized. We find that unidirectional LO states are the most stable mean field solutions in a large range of parameter regimes, and checkerboard order is only clearly favored at small density and large polarization. At lower U , the finite-momentum pairing wave-vector is along $(1, 0)$. We

have shown the insulating versus conducting nature of the nodal region of the superconducting order parameter, and its interplay with commensuration effects. Related to these effects, a new phase with supersolid order is seen when the ordering wave vector is directed along the $(1, 1)$ direction. Our results suggest that, besides time of flight or Bragg spectroscopy, the different phases we discussed are also identifiable by their local density profiles. This, in turn, should help their real-space characterization in the presence of a confining potential.

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